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(FILE 'HOME' ENTERED AT 12:02:23 ON 19 JAN 2004)

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L1 STRUCTURE UPLOADED

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L3 86 S L1 SSS FULL

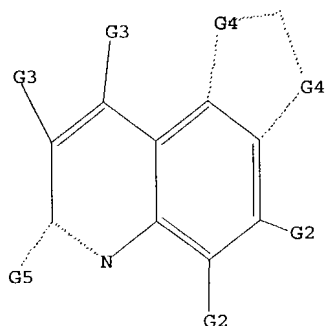
FILE 'CAPLUS' ENTERED AT 12:03:42 ON 19 JAN 2004

L4 23 S L3

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1

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G3 H,O,S,N,Cl,Br,F,I,Me,CH2,CH,CF3,CN

G4 C,N

G5 O,S,N,X,CN

Structure attributes must be viewed using STN Express query preparation.

=> d 1-23 bib abs hitstr

L4 ANSWER 1 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:658121 CAPLUS

DN 137:201294

TI Preparation of pyrroloquinolines, pyridoquinolines, pyranoquinolines, and related tricyclic compounds as androgen receptor modulators

IN Zhi, Lin; Van Oeveren, Cornelis Arjan; Chen, Jyun-Hung; Higuchi, Robert I.

PA Ligand Pharmaceuticals Incorporated, USA

SO PCT Int. Appl., 132 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002066475	A2	20020829	WO 2002-IB537	20020223
WO 2002066475	A3	20030123		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 2002183346	A1	20021205	US 2002-80926	20020222
EP 1363909	A2	20031126	EP 2002-702589	20020223
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
PRAI US 2001-271189P	P	20010223		
WO 2002-IB537	W	20020223		
OS MARPAT 137:201294				
GI				

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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

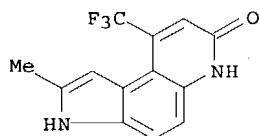
AB Title nonsteroidal tricyclic compds. I-VIII [wherein R1 = H, halo, NO2, OR12, SOO-2R12, NR12R13, or (un)substituted (halo)alkyl or heteroalkyl; R2 = H, halo, Me, CF3, CHF2, CH2F, CF2Cl, CN, CF2OR12, CH2OR12, OR12, SOO-2R12, NR12R13, or (un)substituted (halo)alkyl, heteroalkyl, alkenyl, or alkynyl; R3-R8 = independently H, halo, OR12, NR12R13, SOO-2R12, or (un)substituted (halo)alkyl, heteroalkyl, alkenyl, alkynyl, (hetero)aryl, or arylalkyl; or R3R5 or R5R7 = a bond; or C2R4R6 or C2R6R8 = (un)substituted carbocyclic or heterocyclic ring; R9 and R10 = independently H, halo, CN, OR12, NR12R13, Cm(R12)2mOR13, SOO-2R12, NR12COR13, or (un)substituted (halo)alkyl, heteroalkyl, or arylalkyl; R11 = H, halo, CN, OR14, NR14R15, SOO-2R14, CH2R14, COR14, CO2R14, CONR13R14, or (un)substituted (halo)alkyl or heteroalkyl; R12 and R13 = independently H or (un)substituted (halo)alkyl, heteroalkyl, alkenyl, alkynyl, or (hetero)aryl; R14 = H, COR15, CO2R15, CONR15R16, or (un)substituted (halo)alkyl, heteroalkyl, or (hetero)aryl; R15 and R16 = independently H or (un)substituted (halo)alkyl, or heteroalkyl; W = O or S; X = O, S, or NR14; Y = O, S, NR12, NOR12, or CR12R13; Z = O, S, or NR12; n = 0-2; m = 0-2; or pharmaceutically acceptable salts thereof] were prepd. as modulators of androgen receptors. For example, cyclization of 6-hydrazino-4-trifluoromethylquinolin-2(1H)-one with 3-pentanone afforded the cis-5,6-dihydro-7H-pyrrolo[3,2-f]quinolin-2(1H)-one. Oxidn. with DDQ in CH2Cl2 gave 6-ethyl-5-methyl-7-(2,2,2-trifluoroethyl)-4-trifluoromethyl-1H-pyrrolo[3,2-f]quinolin-2(1H)-one (IX). The latter exhibited 76% androgen receptor agonist efficacy with a potency (EC50) of 7.6 nM relative to dihydrotestosterone in co-transfection assays using CV-1 cells and displayed androgen receptor binding activity (IC50) of 1.7 nM. Pharmaceutical compns. and formulations of IX are also disclosed. I-VIII are useful for the treatment of acne, male-pattern baldness, impotence, sexual dysfunction, wasting disease, hirsutism, hypogonadism, prostatic hyperplasia, osteoporosis, cancer cachexia, and hormone-dependent cancers (no data). Pharmaceutical compns. and formulations of IX are also disclosed.

IT 453592-19-3P 453592-20-6P 453592-22-8P
453592-30-8P 453592-41-1P 453592-46-6P
453592-47-7P 453592-52-4P 453592-53-5P
453592-54-6P 453592-55-7P 453592-56-8P
453592-57-9P 453592-60-4P 453592-71-7P
453592-72-8P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(androgen receptor modulator; prepn. of pyrroloquinolines, pyridoquinolines, pyranoquinolines, and related tricyclic compds. as androgen receptor modulators)

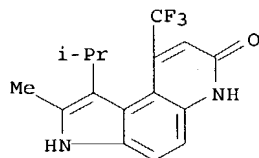
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CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



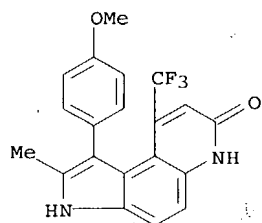
RN 453592-20-6 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-1-(1-methylethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-22-8 CAPLUS

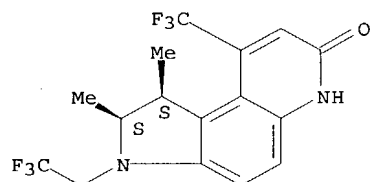
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1-(4-methoxyphenyl)-2-methyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-30-8 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-1,2-dimethyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

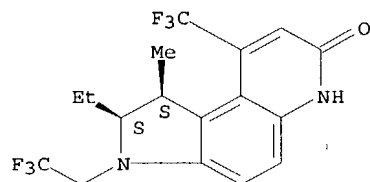
Relative stereochemistry.



RN 453592-41-1 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-1,2,3,6-tetrahydro-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

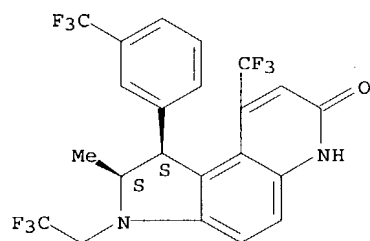
Relative stereochemistry.



RN 453592-46-6 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-1-[3-(trifluoromethyl)phenyl]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

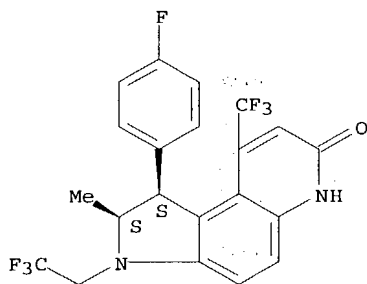
Relative stereochemistry.



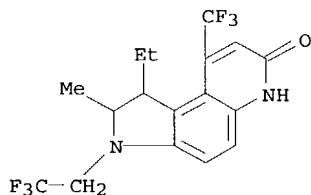
RN 453592-47-7 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-(4-fluorophenyl)-1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

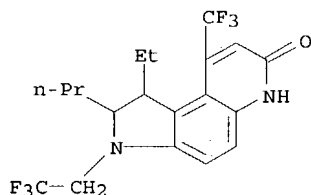
Relative stereochemistry.



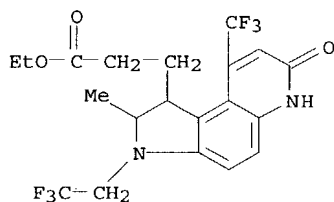
RN 453592-52-4 CAPLUS
 CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-ethyl-1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



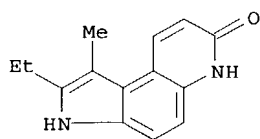
RN 453592-53-5 CAPLUS
 CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-ethyl-1,2,3,6-tetrahydro-2-propyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-54-6 CAPLUS
 CN 1H-Pyrrolo[3,2-f]quinoline-1-propanoic acid, 2,3,6,7-tetrahydro-2-methyl-7-oxo-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)

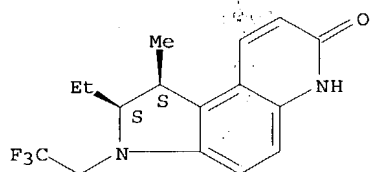


RN 453592-55-7 CAPLUS
 CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-3,6-dihydro-1-methyl- (9CI) (CA INDEX NAME)



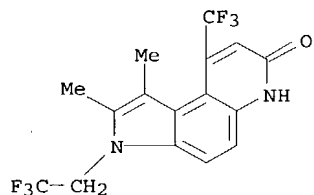
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 CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-1,2,3,6-tetrahydro-1-methyl-3-(2,2,2-trifluoroethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



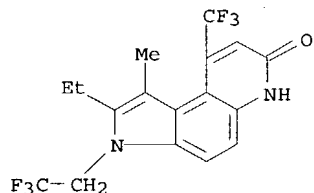
RN 453592-57-9 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2-dimethyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



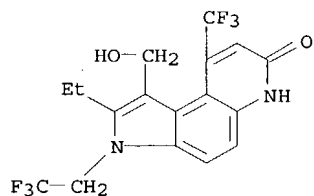
RN 453592-60-4 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-3,6-dihydro-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



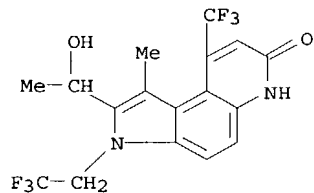
RN 453592-71-7 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-3,6-dihydro-1-(hydroxymethyl)-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-72-8 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-(1-hydroxyethyl)-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



IT 453592-21-7P 453592-23-9P 453592-42-2P
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453592-48-8P 453592-49-9P 453592-50-2P

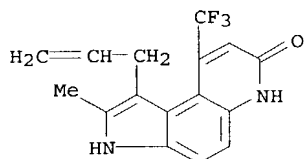
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 453592-77-3P 453592-78-4P 453592-79-5P
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 453592-84-2P 453593-25-4P 453593-26-5P
 453593-30-1P 453593-31-2P 453593-32-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(androgen receptor modulator; prepn. of pyrroloquinolines,
 pyridoquinolines, pyranoquinolines, and related tricyclic compds. as
 androgen receptor modulators)

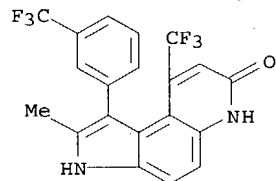
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CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-1-(2-propenyl)-9-
 (trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-23-9 CAPLUS

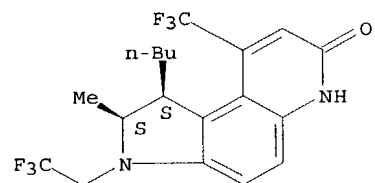
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-9-(trifluoromethyl)-
 1-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 453592-42-2 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-butyl-1,2,3,6-tetrahydro-2-methyl-3-
 (2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX
 NAME)

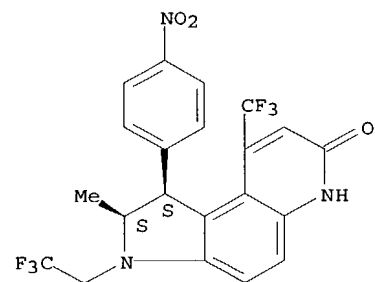
Relative stereochemistry.

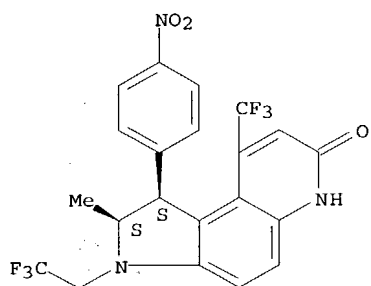


RN 453592-43-3 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-2-methyl-1-(4-
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 (9CI) (CA INDEX NAME)

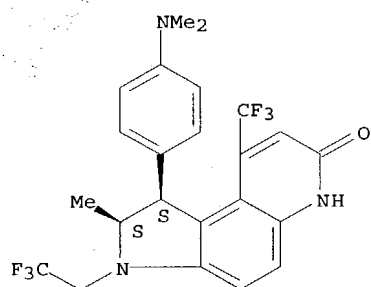
Relative stereochemistry.





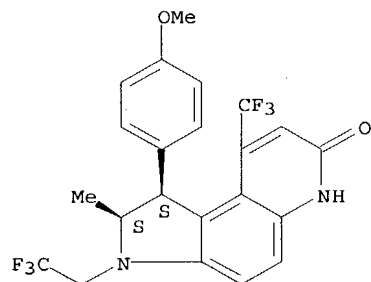
RN 453592-44-4 CAPLUS
 CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-[4-(dimethylamino)phenyl]-1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

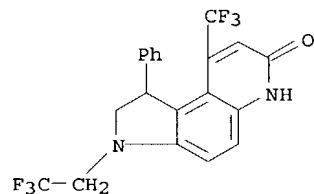


RN 453592-45-5 CAPLUS
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Relative stereochemistry.

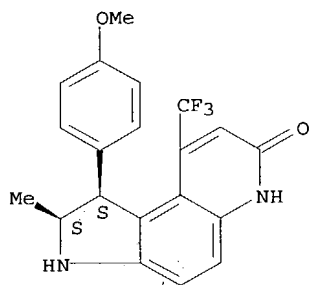


RN 453592-48-8 CAPLUS
 CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-1-phenyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



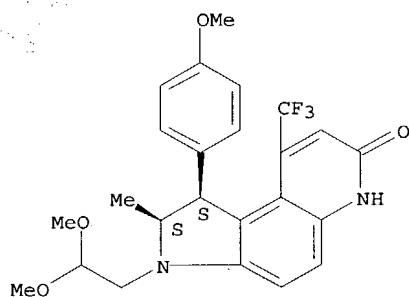
RN 453592-49-9 CAPLUS
 CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-1-(4-methoxyphenyl)-2-methyl-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



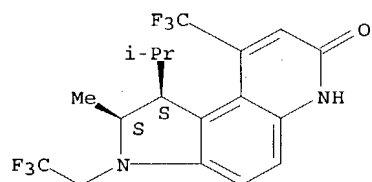
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 CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3-(2,2-dimethoxyethyl)-1,2,3,6-tetrahydro-1-(4-methoxyphenyl)-2-methyl-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

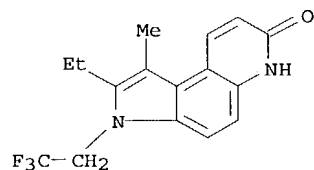


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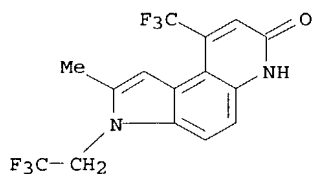
Relative stereochemistry.



RN 453592-58-0 CAPLUS
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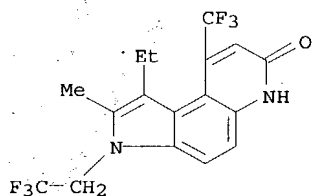


RN 453592-59-1 CAPLUS
 CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



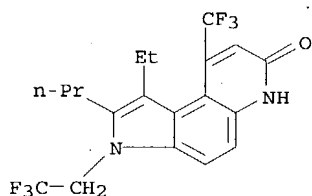
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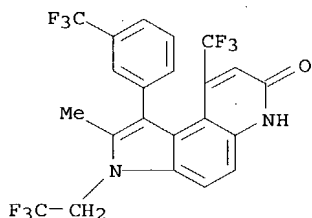
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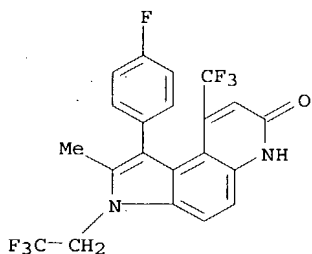
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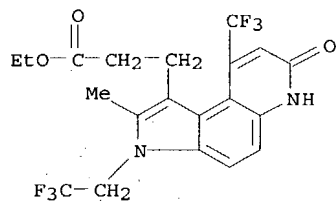
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-(4-fluorophenyl)-3,6-dihydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-69-3 CAPLUS

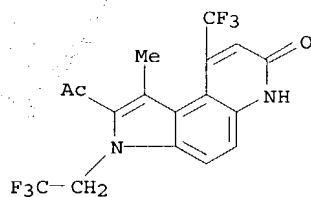
CN 3H-Pyrrolo[3,2-f]quinoline-1-propanoic acid, 6,7-dihydro-2-methyl-7-oxo-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)



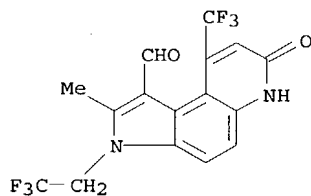
RN 453592-73-9 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-acetyl-3,6-dihydro-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



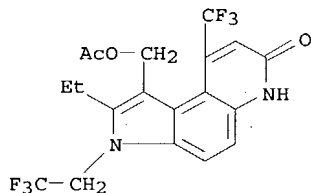
RN 453592-74-0 CAPLUS

CN 3H-Pyrrolo[3,2-f]quinoline-1-carboxaldehyde, 6,7-dihydro-2-methyl-7-oxo-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



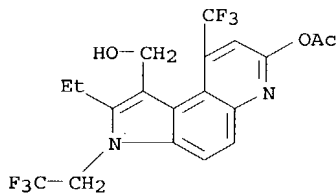
RN 453592-75-1 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-[(acetyloxy)methyl]-2-ethyl-3,6-dihydro-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



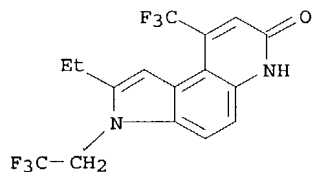
RN 453592-76-2 CAPLUS

CN 3H-Pyrrolo[3,2-f]quinoline-1-methanol, 7-(acetyloxy)-2-ethyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



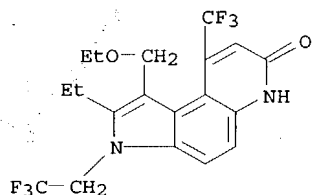
RN 453592-77-3 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-3,6-dihydro-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



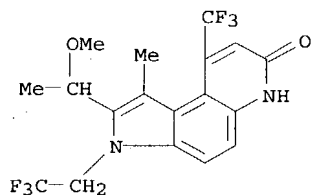
RN 453592-78-4 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-(ethoxymethyl)-2-ethyl-3,6-dihydro-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



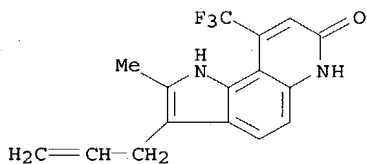
RN 453592-79-5 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-(1-methoxyethyl)-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



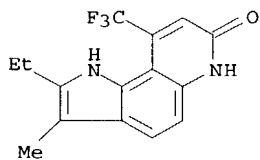
RN 453592-80-8 CAPLUS

CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 1,6-dihydro-2-methyl-3-(2-propenyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



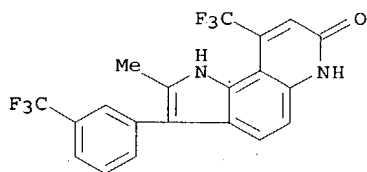
RN 453592-82-0 CAPLUS

CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 2-ethyl-1,6-dihydro-3-methyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

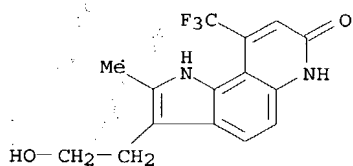


RN 453592-83-1 CAPLUS

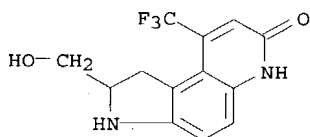
CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 1,6-dihydro-2-methyl-9-(trifluoromethyl)-3-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



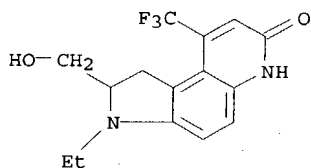
RN 453592-84-2 CAPLUS
 CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 1,6-dihydro-3-(2-hydroxyethyl)-2-methyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



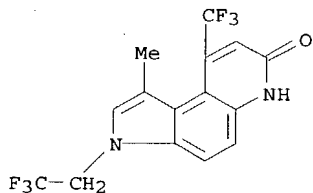
RN 453593-25-4 CAPLUS
 CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-2-(hydroxymethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



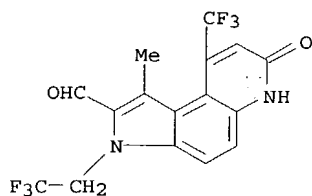
RN 453593-26-5 CAPLUS
 CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3-ethyl-1,2,3,6-tetrahydro-2-(hydroxymethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



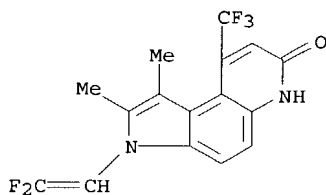
RN 453593-30-1 CAPLUS
 CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



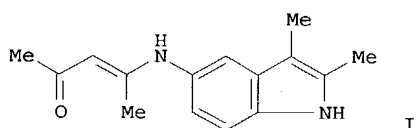
RN 453593-31-2 CAPLUS
 CN 3H-Pyrrolo[3,2-f]quinoline-2-carboxaldehyde, 6,7-dihydro-1-methyl-7-oxo-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



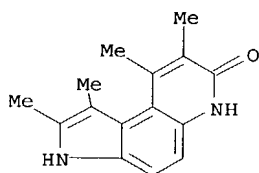
RN 453593-32-3 CAPLUS
 CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3-(2,2-difluoroethenyl)-3,6-dihydro-1,2-dimethyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



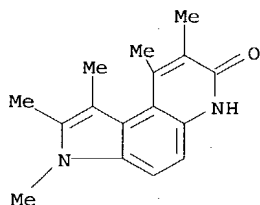
L4 ANSWER 2 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1999:455695 CAPLUS
 DN 131:213835
 TI Reactivities of 5-, 6-, and 7-(enamino)indoles in the synthesis of pyrroloquinolines
 AU Yamashkin, S. A.; Trushkov, I. V.; Tomilin, O. B.; Terekhin, I. I.; Yurovskaya, M. A.
 CS Mordovian State Pedagogical Institute, Saransk, 430007, Russia
 SO Chemistry of Heterocyclic Compounds (New York) (Translation of Khimiya Geterotsiklicheskikh Soedinenii) (1999), Volume Date 1998, 34(9), 1050-1065
 CODEN: CHCCAL; ISSN: 0009-3122
 PB Consultants Bureau
 DT Journal
 LA English
 GI



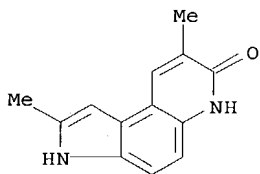
AB The concept of regioorientation is proposed for the annelation of the pyridine ring with the participation of 5-, 6-, and 7-aminoindoles (e.g., I). The conclusions based on the exptl. data are supported by semiempirical AM1, PM3, and MNDO quantum-chem. calcns.
 IT 243669-00-3 243669-02-5 243669-04-7
 243669-06-9
 RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
 (reactivities of 5-, 6-, and 7-(enamino)indoles in the synthesis of pyrroloquinolines)
 RN 243669-00-3 CAPLUS
 CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2,8,9-tetramethyl- (9CI) (CA INDEX NAME)



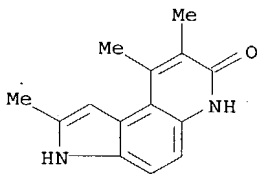
RN 243669-02-5 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2,3,8,9-pentamethyl- (9CI)
(CA INDEX NAME)



RN 243669-04-7 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2,8-dimethyl- (9CI) (CA
INDEX NAME)

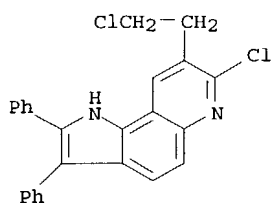


RN 243669-06-9 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2,8,9-trimethyl- (9CI) (CA
INDEX NAME)



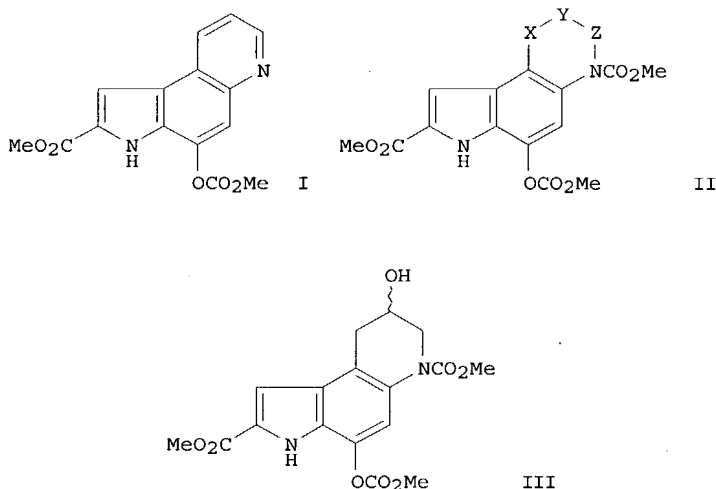
RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:731923 CAPLUS
DN 130:13934
TI Synthesis of pyrrolo-, thienopyrrolo-, and benzothienopyrroloquinolines as
well as of triazoloindole derivatives
AU El-Desoky, S. I.; Kandeel, E. M.; Abd El-Rahman, A. H.; Shmidt, R. R.
CS Chemistry Department, Faculty Science, Mansoura University, Mansoura,
Egypt
SO Zeitschrift fuer Naturforschung, B: Chemical Sciences (1998), 53(10),
1216-1222
CODEN: ZNBSEN; ISSN: 0932-0776
PB Verlag der Zeitschrift fuer Naturforschung
DT Journal
LA English
OS CASREACT 130:13934
AB Pyrroloquinolines, thienopyrroloquinolines, benzothienopyrroloquinolines,
and triazoloindoles were prepd. starting from 6-amino-2,3-diphenylindole.
IT 216073-29-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. of pyrroloquinolines, thienopyrroloquinolines,
benzothienopyrroloquinolines, and triazoloindoles)
RN 216073-29-9 CAPLUS
CN 1H-Pyrrolo[2,3-f]quinoline, 7-chloro-8-(2-chloroethyl)-2,3-diphenyl- (9CI)
(CA INDEX NAME)

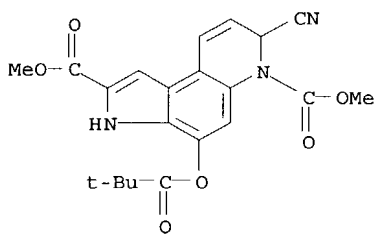


RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:226505 CAPLUS
DN 128:294622
TI Synthesis of duocarmycin SA by way of methyl 4-(methoxycarbonyl)oxy-3H-pyrrolo[3,2-f]quinoline-2-carboxylate as a tricyclic heteroaromatic intermediate
AU Muratake, Hideaki; Tonegawa, Miyuki; Natsume, Mitsutaka
CS Research Foundation Itsuu Laboratory, Tokyo, 158, Japan
SO Chemical & Pharmaceutical Bulletin (1998), 46(3), 400-412
CODEN: CPBTAL; ISSN: 0009-2363
PB Pharmaceutical Society of Japan
DT Journal
LA English
OS CASREACT 128:294622
GI



AB The new synthetic path proposed that a fully arom. I would afford the dihydropyridine deriv. II (X=Y = CH=CH, Z = CH2; X = CH2, Y=Z = CH=CH) on partial redn. and by making use of the double bonds formed, a hydroxyl group could be introduced at the required position either in a racemic or in an asym. way to yield III. The Stille coupling product obtained from the bromopyrrole with the stannylpyridine represented a potential precursor. Both Sharpless asym. dihydroxylation (AD) and Jacobsen's asym. epoxidn. were applied to II (X=Y = CH=CH, Z = CH2; X = CH2, Y=Z = CH=CH). At the best, 81% ee was obsd. in the AD reaction of II (X=Y = CH=CH, Z = CH2) using 2,5-diphenyl-4,6-bis(9-O-dihydroquinyl)pyrimidine [(DHQ)2PYP], but the product possessed an unnatural abs. configuration. Formal syntheses of (.-.)-duocarmycin SA, natural (+)-duocarmycin SA and unnatural (-)-duocarmycin SA were accomplished via a tricyclic heteroarom. compd. I.
IT 206115-56-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of duocarmycin SA via the tricyclic heteroarom. intermediate Me 4-(methoxycarbonyl)oxy-3H-pyrrolo[3,2-f]quinoline-2-carboxylate)
RN 206115-56-2 CAPLUS
CN 6H-Pyrrolo[3,2-f]quinoline-2,6-dicarboxylic acid, 7-cyano-4-(2,2-dimethyl-1-oxopropoxy)-3,7-dihydro-, dimethyl ester (9CI) (CA INDEX NAME)

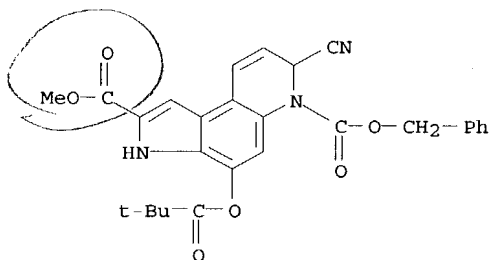


IT 206115-76-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of duocarmycin SA via the tricyclic heteroarom. intermediate Me
4-(methoxycarbonyl)oxy-3H-pyrrolo[3,2-f]quinoline-2-carboxylate)

RN 206115-76-6 CAPLUS

CN 6H-Pyrrolo[3,2-f]quinoline-2,6-dicarboxylic acid, 7-cyano-4-(2,2-dimethyl-
1-oxopropoxy)-3,7-dihydro-, 2-methyl 6-(phenylmethyl) ester (9CI) (CA
INDEX NAME)



RE.CNT 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1997:698152 CAPLUS

DN 128:3621

TI Studies on amine oxide rearrangements: regioselective synthesis of
pyrrolo[3,2-f]quinolin-7-ones

AU Majumdar, Krishna C.; Biswas, Paritosh; Jana, Gour H.

CS Dep. Chem., Univ. Kalyani, Kalyani, 741 235, India

SO Journal of Chemical Research, Synopses (1997), (9), 310-311

CODEN: JRPSDC; ISSN: 0308-2342

PB Royal Society of Chemistry

DT Journal

LA English

OS CASREACT 128:3621

AB A no. of derivs. of the hitherto unreported pyrrolo[3,2-f]quinolin-7-one
tricyclic system have been synthesized from 6-nitroquinolone by successive
redn., tosylation, methylation, detosylation, prop-2-ynylation, and
treatment with m-chloroperoxybenzoic acid.

IT 198639-83-7P 198639-84-8P 198639-85-9P

198639-86-0P 198639-87-1P 198639-88-2P

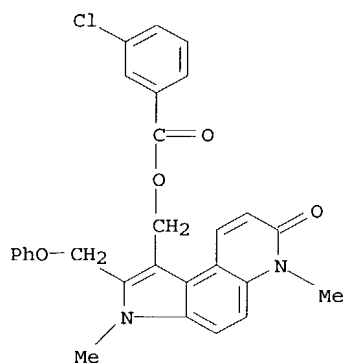
198639-90-6P 198640-00-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(regioselective prepn. of pyrrolo[3,2-f]quinolin-7-ones)

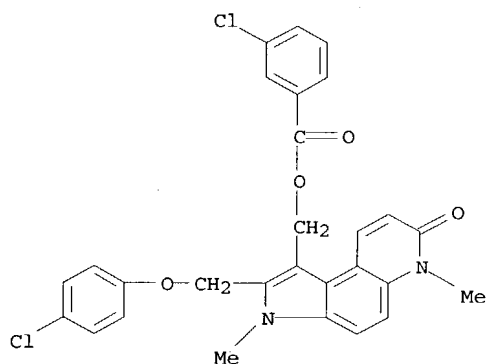
RN 198639-83-7 CAPLUS

CN Benzoic acid, 3-chloro-, [6,7-dihydro-3,6-dimethyl-7-oxo-2-(phenoxymethyl)-
3H-pyrrolo[3,2-f]quinolin-1-yl]methyl ester (9CI) (CA INDEX NAME)



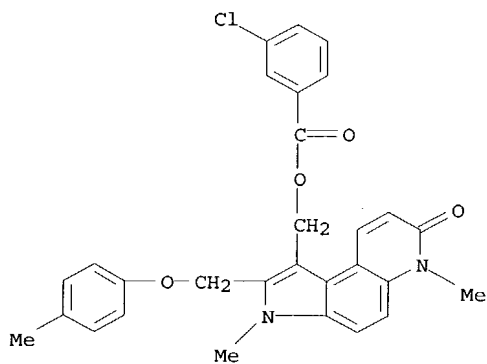
RN 198639-84-8 CAPLUS

CN Benzoic acid, 4-chloro-, [2-[(4-chlorophenoxy)methyl]-6,7-dihydro-3,6-dimethyl-7-oxo-3H-pyrrolo[3,2-f]quinolin-1-yl]methyl ester (9CI) (CA INDEX NAME)



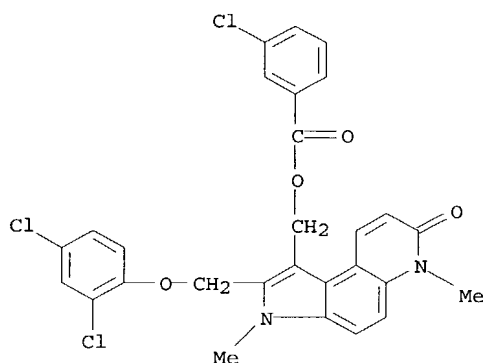
RN 198639-85-9 CAPLUS

CN Benzoic acid, 3-chloro-, [6,7-dihydro-3,6-dimethyl-2-[(4-methylphenoxy)methyl]-7-oxo-3H-pyrrolo[3,2-f]quinolin-1-yl]methyl ester (9CI) (CA INDEX NAME)

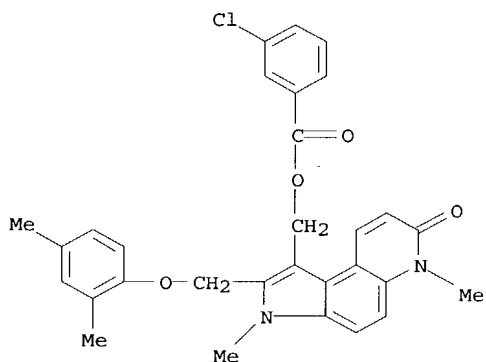


RN 198639-86-0 CAPLUS

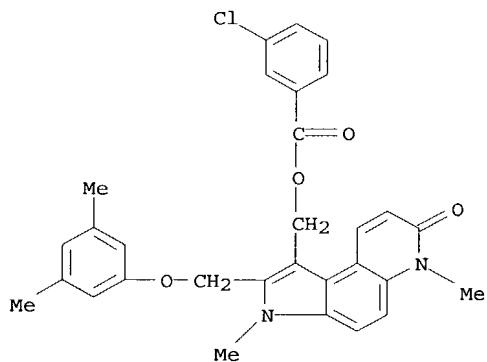
CN Benzoic acid, 3-chloro-, [2-[(2,4-dichlorophenoxy)methyl]-6,7-dihydro-3,6-dimethyl-7-oxo-3H-pyrrolo[3,2-f]quinolin-1-yl]methyl ester (9CI) (CA INDEX NAME)



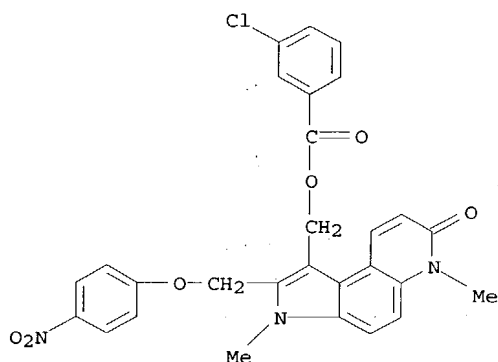
RN 198639-87-1 CAPLUS
 CN Benzoic acid, 3-chloro-, [2-[(2,4-dimethylphenoxy)methyl]-6,7-dihydro-3,6-dimethyl-7-oxo-3H-pyrrolo[3,2-f]quinolin-1-yl)methyl ester (9CI) (CA INDEX NAME)



RN 198639-88-2 CAPLUS
 CN Benzoic acid, 3-chloro-, [2-[(3,5-dimethylphenoxy)methyl]-6,7-dihydro-3,6-dimethyl-7-oxo-3H-pyrrolo[3,2-f]quinolin-1-yl)methyl ester (9CI) (CA INDEX NAME)

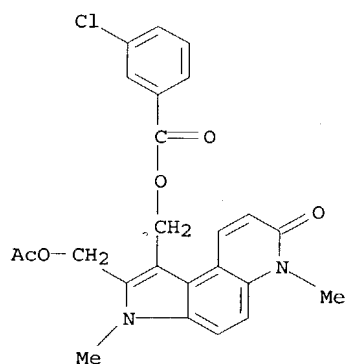


RN 198639-90-6 CAPLUS
 CN Benzoic acid, 3-chloro-, [6,7-dihydro-3,6-dimethyl-2-[(4-nitrophenoxy)methyl]-7-oxo-3H-pyrrolo[3,2-f]quinolin-1-yl)methyl ester (9CI) (CA INDEX NAME)



RN 198640-00-5 CAPLUS

CN Benzoic acid, 3-chloro-, [2-[(acetyloxy)methyl]-6,7-dihydro-3,6-dimethyl-7-oxo-3H-pyrrolo[3,2-f]quinolin-1-yl]methyl ester (9CI) (CA INDEX NAME)



IT 198639-91-7P 198639-92-8P 198639-94-0P

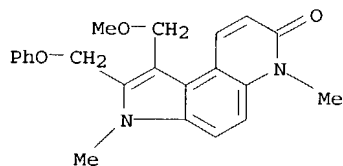
198639-95-1P 198639-96-2P 198639-97-3P

198639-98-4P 198640-01-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective prepn. of pyrrolo[3,2-f]quinolin-7-ones)

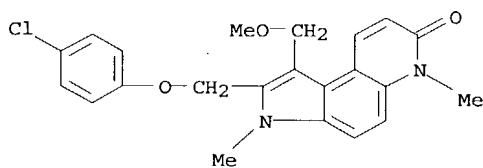
RN 198639-91-7 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1-(methoxymethyl)-3,6-dimethyl-2-(phenoxymethyl)- (9CI) (CA INDEX NAME)



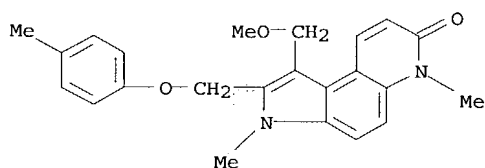
RN 198639-92-8 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-[(4-chlorophenoxy)methyl]-3,6-dihydro-1-(methoxymethyl)-3,6-dimethyl- (9CI) (CA INDEX NAME)



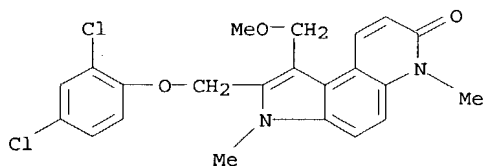
RN 198639-94-0 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1-(methoxymethyl)-3,6-dimethyl-2-[(4-methylphenoxy)methyl]- (9CI) (CA INDEX NAME)



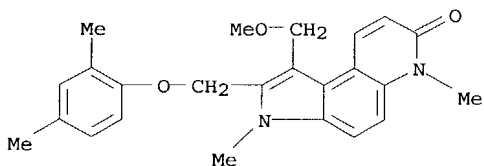
RN 198639-95-1 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-[(2,4-dichlorophenoxy)methyl]-3,6-dihydro-1-(methoxymethyl)-3,6-dimethyl- (9CI) (CA INDEX NAME)



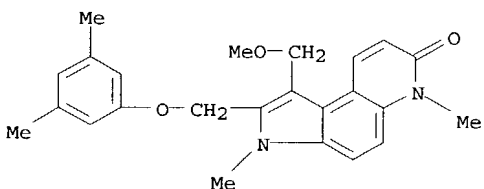
RN 198639-96-2 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-[(2,4-dimethylphenoxy)methyl]-3,6-dihydro-1-(methoxymethyl)-3,6-dimethyl- (9CI) (CA INDEX NAME)



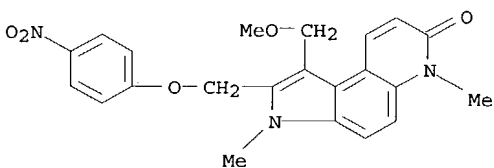
RN 198639-97-3 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-[(3,5-dimethylphenoxy)methyl]-3,6-dihydro-1-(methoxymethyl)-3,6-dimethyl- (9CI) (CA INDEX NAME)



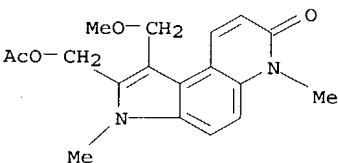
RN 198639-98-4 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1-(methoxymethyl)-3,6-dimethyl-2-[(4-nitrophenoxy)methyl]- (9CI) (CA INDEX NAME)



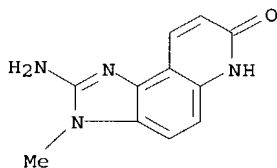
RN 198640-01-6 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-[(acetyloxy)methyl]-3,6-dihydro-1-(methoxymethyl)-3,6-dimethyl- (9CI) (CA INDEX NAME)



RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:839604 CAPLUS
DN 123:248961
TI Dietary modulation of the carcinogenicity of the heterocyclic amines
AU Weisburger, J. H.; Rivenson, A.; Kingston, D. G. I.; Wilkins, T. D.; Van
Tassell, R. L.; Nagao, M.; Sugimura, T.; Hara, Y.
CS American Health Foundation, Valhalla, NY, 10595, USA
SO Proceedings of the International Symposium of the Princess Takamatsu
Cancer Research Fund (1995), Volume Date 1992, 23rd(Heterocyclic Amines in
Cooked Foods: Possible Human Carcinogens), 240-50
CODEN: PPTCBY
PB Princeton Scientific
DT Journal
LA English
AB A series of studies explore modulation of the mutagenicity and
carcinogenicity of typical HCAs like 2-amino-3-methylimidazo[4,5-
f]quinoline (IQ), and of 2-amino-1-methyl-6-phenylimidazo[4,5-b]pyridine
(PhIP), through dietary fat, green or black tea, and tea polyphenols like
epigallocatechin gallate (EGCG) and theaflavin gallate (TFG). Also examd.
was the carcinogenicity of the bacterial metabolite of IQ, 7-oxo-IQ. Male
and female F344 rats were fed diets with 75 ppm IQ for 12 mo, and contg.
5% or 20% corn oil. Complete necropsies after 15 mo (males), or 18 mo
(females) were performed. Modification of the action of IQ and of PhIP in
tests for bacterial mutagenicity (Ames test) or DNA repair in male rat
hepatocytes (Williams test) by teas, EGCG or TFG was studied. Also
compared was the activity of IQ and of 7-oxo-IQ in the tests of Ames and
of Williams, and their carcinogenicity in male F344 rats upon intrarectal
infusion. A high fat diet was found to increase the carcinogenicity of
low levels of IQ at several target organs. Multiple benign and malignant
sebaceous skin tumors were noted in males but not in females. Green or
black teas, EGCG, and TFG sharply reduced the mutagenicity of IQ and PhIP,
and esp. lowered the activity of IQ and of PhIP in the Williams test.
7-Oxo-IQ was active only in the Ames test, but not in the Williams test.
Also, it was not carcinogenic, confirming that chems. pos. in the Ames
test but neg. in the Williams test are not likely carcinogens. The in
vitro and in vivo effects of HCAs can be modified by dietary components
such as fats or teas.
IT 108043-88-5, 7-Oxo-IQ
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(carcinogenicity of heterocyclic amines)
RN 108043-88-5 CAPLUS
CN 7H-Imidazo[4,5-f]quinolin-7-one, 2-amino-3,6-dihydro-3-methyl- (9CI) (CA
INDEX NAME)



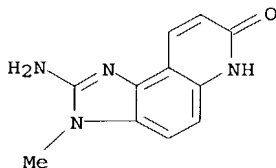
L4 ANSWER 7 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1994:551041 CAPLUS
DN 121:151041
TI Genotoxicity and carcinogenicity in rats and mice of 2-amino-3,6-dihydro-3-
methyl-7H-imidazolo[4,5-f]quinolin-7-one: an intestinal bacterial
metabolite of 2-amino-3-methyl-3H-imidazo[4,5-f]quinoline
AU Weisburger, John H.; Rivenson, Abraham; Reinhardt, Joel; Aliaga, Cesar;
Braley, Joanne; Dolan, Lisa M.; Williams, Gary M.; Zang, Edith; Kingston,
David G. I.; et al.
CS Am. Health Found., Valhalla, NY, 10595, USA
SO Journal of the National Cancer Institute (1994), 86(1), 25-30
CODEN: JNCIEQ; ISSN: 0027-8874
DT Journal
LA English
AB The authors confirmed that 2-amino-3,6-dihydro-3-methyl-7H-imidazolo[4,5-
f]quinolin-7-one (7-OHIQ) is a direct-acting mutagen in the Ames test,
with added S9 liver fraction giving higher mutagenicity. 7-OHIQ was neg.
in the Williams test, whereas IQ was pos. 7-OHIQ did not induce colon
cancer in rats, and in the newborn mouse test it produced only a low
incidence of liver neoplasms. Apparently, 7-OHIQ is not genotoxic, for to
be so classified it must be definitely pos. in both the Ames and Williams

tests; moreover, it is not carcinogenic, in marked contrast to IQ and NMU.

IT 108043-88-5
 RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
 (carcinogenicity and mutagenicity of)

RN 108043-88-5 CAPLUS

CN 7H-Imidazo[4,5-f]quinolin-7-one, 2-amino-3,6-dihydro-3-methyl- (9CI) (CA
 INDEX NAME)



L4 ANSWER 8 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1993:648896 CAPLUS

DN 119:248896

TI Influence of diet on the conversion of 2-amino-3-methyl-3H-imidazo[4,5f]quinoline (IQ) to the 7-keto derivative (7-OHIQ)

AU Rumney, C. J.; Rowland, I. R.

CS BIBRA Toxicol. Int., Carshalton/Surrey, SM5 4DS, UK

SO Special Publication - Royal Society of Chemistry (1993), 123(Food and Cancer Prevention: Chemical and Biological Aspects), 70-4
 CODEN: SROCDQ; ISSN: 0260-6291

DT Journal

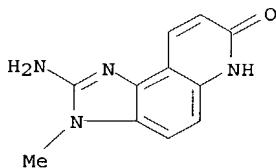
LA English

AB The effect of dietary fats, fiber, and transgalactosylated oligosaccharides (TOS) on the conversion of a carcinogen IQ to a direct-acting genotoxin, 7-hydroxy-2-amino-3,6-dihydro-3-methyl-3H-imidazo[4,5-f]quinoline-7-one (7-OHIQ), by human gut bacteria was studied on rats adapted to human gut bacteria. After 18-h incubation of ¹⁴C-labeled IQ with cecal content from rats fed a diet contg. 1% fat or 25% fat as beef drippings, about 95% IQ was converted into 7-OHIQ, whereas this conversion amounted 65% only when rats were fed a diet contg 25% olive oil. No significant differences in the rate of conversion was found during 24-h incubation of cecal contents from rats fed a dietary fiber-free diet in comparison with diets contg. dietary fiber from sugar beet, wheat bran, and oats. In rats supplemented with TOS, the conversion of IQ to 7-OHIQ was restricted to 77% in comparison with 93% in the cecal content from unsupplemented control rats.

IT 108043-88-5
 RL: BIOL (Biological study)
 (IQ conversion to, by cecal microflora, dietary factors affecting, carcinogenicity and genotoxicity in relation to)

RN 108043-88-5 CAPLUS

CN 7H-Imidazo[4,5-f]quinolin-7-one, 2-amino-3,6-dihydro-3-methyl- (9CI) (CA
 INDEX NAME)



L4 ANSWER 9 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1993:648895 CAPLUS

DN 119:248895

TI Influence of dietary fat on metabolism of 2-amino-3-methyl-3H-imidazo[4,5-f]quinoline (IQ)

AU Rumney, C. J.; Rowland, I. R.; O'Neill, I. K.

CS BIBRA Toxicol. Int., Carshalton/Surrey, SM5 4DS, UK

SO Special Publication - Royal Society of Chemistry (1993), 123(Food and Cancer Prevention: Chemical and Biological Aspects), 65-9
 CODEN: SROCDQ; ISSN: 0260-6291

DT Journal

LA English

AB The potential effect of low- vs. high-fat diets on the metab. of IQ was studied on human flora-assocd. rats fed human diets. The risk assocd.

with ingestion of a pyrolysis carcinogen, such as IQ, may be reduced by a decrease in dietary fat level. Thus, on the low-fat diet as compared with the high-fat diet, the in vitro hepatic activation of IQ was 230 vs. 530 revertants per plate; the conversion of IQ to 7-hydroxy-IQ by cecal content during 6-h incubation was 10 vs. 30%; and the activity of .beta.-glucuronidase in the cecal content was 10 vs. 50 .mu.mol/h/g.

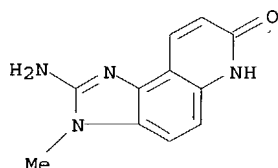
IT 108043-88-5

RL: FORM (Formation, nonpreparative)

(formation of, in IQ metab. in cecal content, dietary fat level effect on, carcinogenicity in relation to)

RN 108043-88-5 CAPLUS

CN 7H-Imidazo[4,5-f]quinolin-7-one, 2-amino-3,6-dihydro-3-methyl- (9CI) (CA INDEX NAME)



L4 ANSWER 10 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1993:556798 CAPLUS

DN 119:156798

TI Conversion of IQ to 7-OHIQ by gut microflora

AU Rumney, Corinne J.; Rowland, Ian R.; O'Neill, Ian K.

CS BIBRA Toxicol. Int., Carshalton/Surrey, SM5 4DS, UK

SO Nutrition and Cancer (1993), 19(1), 67-76

CODEN: NUCADQ; ISSN: 0163-5581

DT Journal

LA English

AB The rates of conversion of 2-amino-3-methyl-3H-imidazo[4,5-f]quinoline (IQ) to its reportedly mutagenic 7-keto deriv. (7-OHIQ) by intestinal bacteria from humans, mice, and rats were compared. IQ was metabolized faster by cecal contents from rats or mice than by human fecal samples (113 and 87 .mu.mol 7-OHIQ formed/h-g cecal contents, resp., vs. 12.3 .mu.mol/h-g feces). Cecal contents from germ-free rats colonized with human fecal bacteria [human flora-assocd. (HFA) rats] converted IQ to 7-OHIQ at rates generally lower than contents from rats colonized with their native flora. Diet had a marked effect on IQ metab. by HFA rat cecal contents. The rate of IQ conversion to 7-OHIQ was increased in rats fed on a diet high in beef dripping compared with that in rats fed a low-fat control diet. A diet high in olive oil, however, did not produce an increase in the IQ conversion rate. Addn. of fiber to a purified diet increased the rate of IQ metab. in the following order: sugar beet fiber > wheat bran > oat bran fiber > fiber-free diet. In a further study, HFA rats were fed human diets altered independently in their fat, fiber (wheat bran), and beef contents. The high-fiber diet produced the greatest increase in IQ conversion rate, followed by the high-fat diet. The diet with a high beef content and the control diet (low levels of all 3 macrocomponents) produced similarly low rates of IQ conversion. Material from incubations of IQ with HFA rat cecal contents, assumed to be 7-OHIQ on the basis of chromatog. behavior, was confirmed to be directly mutagenic, producing .apprx.800 His+ revertants/.mu.g with S. typhimurium TA98.

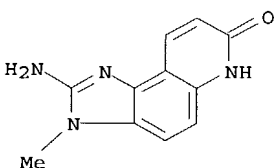
IT 108043-88-5

RL: FORM (Formation, nonpreparative)

(formation of, from IQ by intestinal microorganisms, diet effect on)

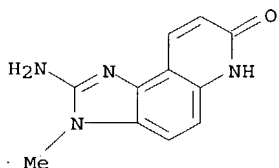
RN 108043-88-5 CAPLUS

CN 7H-Imidazo[4,5-f]quinolin-7-one, 2-amino-3,6-dihydro-3-methyl- (9CI) (CA INDEX NAME)

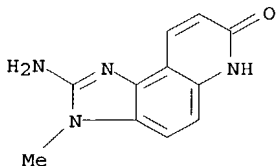


L4 ANSWER 11 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1993:516159 CAPLUS
 DN 119:116159
 TI Effect of diet on glucuronide hydrolysis and the conversion of IQ to 7-OHIQ by caecal contents of human flora associated (HFA) rats
 AU Rumney, Corinne; Rowland, Ian; Shah, Atul; Ellul, Ann; O'Neill, Ian
 CS BIBRA, Carshalton/Surrey, SM5 4DS, UK
 SO Mikrooekologie und Therapie (1992), 20(Exp. Klin. Gnotobiol.), 107-10
 CODEN: MITHE4; ISSN: 0720-0536
 DT Journal
 LA English
 AB High-fat and high-fiber diets gave greatest conversion of 2-amino-3-methyl-3H-imidazo[4,5-f]quinoline(IQ) to 7-hydroxy-2-amino-3,6-dihydro-3-methyl-7H-imidazo[4,5-f]quinoline-7-one (7-OHIQ) in rats with human cecal flora. Germ-free rats showed no conversion. The high-fat group had highest .beta.-glucuronidase activity, followed by the high-fiber and then high-beef and low-fiber,fat,beef groups.
 IT 108043-88-5
 RL: FORM (Formation, nonpreparative)
 (formation of, by cecal bacteria, diet compn. effect on)
 RN 108043-88-5 CAPLUS
 CN 7H-Imidazo[4,5-f]quinolin-7-one, 2-amino-3,6-dihydro-3-methyl- (9CI) (CA INDEX NAME)



L4 ANSWER 12 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1993:249678 CAPLUS
 DN 118:249678
 TI Prostaglandin H synthase-dependent formation of the direct-acting mutagen 2-nitro-3-methylimidazo[4,5-f]quinoline (nitro-IQ) from IQ
 AU Morrison, Lesley D.; Eling, Thomas E.; Josephy, P. David
 CS Guelph-Waterloo Cent. Grad. Work Chem., Univ. Guelph, Guelph, ON, N1G 2W1, Can.
 SO Mutation Research (1993), 302(1), 45-52
 CODEN: MUREAV; ISSN: 0027-5107
 DT Journal
 LA English
 AB The mutagenic effects of IQ following activation by ram seminal vesicle microsomes (RSVM, a source of prostaglandin H synthase, PHS) were studied in Salmonella typhimurium tester strains possessing elevated levels of acetyl-CoA:arylamine N-acetyltransferase (NAT). The metabolites formed by RSVM were extd. and fractionated by HPLC. One isolable product accounted for most of the direct-acting mutagenicity obsd. in the exts. The metabolite was identified as nitro-IQ.
 IT 108043-88-5
 RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
 (mutagenicity of)
 RN 108043-88-5 CAPLUS
 CN 7H-Imidazo[4,5-f]quinolin-7-one, 2-amino-3,6-dihydro-3-methyl- (9CI) (CA INDEX NAME)

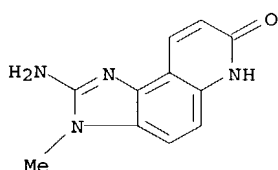


L4 ANSWER 13 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1993:75141 CAPLUS
 DN 118:75141
 TI Entrapment by magnetic microcapsules of the protein pyrolysates IQ, PhIP and Glu-P-1, and alteration of IQ metabolite exposure within the rat gastrointestinal tract by risk-modulating components of the human diet
 AU O'Neill, I.; Ohgaki, H.; Ellul, A.; Turesky, R. J.

CS Int. Agency Res. Cancer, Lyon, 69372, Fr.
 SO Carcinogenesis (1992), 13(12), 2353-9
 CODEN: CRNGDP; ISSN: 0143-3334
 DT Journal
 LA English
 AB The entrapment of heterocyclic arom. amine gastrointestinal carcinogens (HAAs), by retrievable semipermeable magnetic polyethyleneimine (PEI) microcapsules was investigated in vitro and in vivo as an approach for human biomonitoring. The 14C-labeled IQ, PhIP and Glu-P-1 are adsorbed to PEI microcapsules in vitro and can be desorbed by treatment with methanolic ammonia. Binding of HAAs to PEI microcapsules contg. copper phthalocyanine, a moiety which reversibly binds chems. with arom. planar structures, was 2- to 4-fold higher than with unmodified PEI microcapsules. PEI microcapsules also acted as a nucleophile and trapped the proximate carcinogenic metabolite of IQ, N-hydroxy-IQ. The entrapment of 14C-labeled IQ and PhIP by microcapsules was investigated in vivo in male F344 rats fed a conventional chow diet or a human diet with varying amts. of fat and beef intake typically consumed in the UK. Animals were adapted to human diets which were either high (H) or low (L) in fat (F), beef protein (B) and dietary fiber non-starch polysaccharide (NSP). Microcapsule entrapment of IQ and metabolites was 0.5-2.0% of the dose and 4-fold higher in rats consuming a HF/HB/LNSP than those consuming a LF/LB/HNSP diet, these being resp. putative high- and low-risk-assocd. diets. In the HF/HB/LNSP diet group, a higher amt. of IQ metabolites were detected in the microcapsules; a lower proportion of covalently bound metabolites could be removed by acid hydrolysis. Urinary excretion was 2-fold greater and anal. of the urinary metabolites showed there to be lower sulfotransferase activity than in the LF/LB/HNSP group. The amt. of 14C-labeled PhIP entrapped by PEI microcapsules was 1.5% of the dose in rodents fed a LF/HB/LNSP human diet and binding was 7-fold higher than in rodents fed a semi-purified diet. These results demonstrate that microcapsules can entrap IQ and PhIP and their metabolites within the GI tract of rodents. The amts. entrapped by microcapsules in the rodent model suggest that this approach may be feasible for human biomonitoring of HAAs and for non-invasively studying dietary modulations of carcinogen exposure within a potential HAA target organ at high risk from as-yet unidentified causes.

IT 108043-88-5
 RL: BIOL (Biological study)
 (IQ metabolite, factors affecting metab. from magnetic microcapsules in relation to)

RN 108043-88-5 CAPLUS
 CN 7H-Imidazo[4,5-f]quinolin-7-one, 2-amino-3,6-dihydro-3-methyl- (9CI) (CA INDEX NAME)



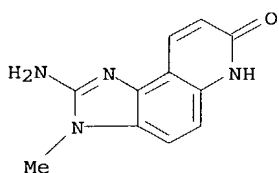
L4 ANSWER 14 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1992:632345 CAPLUS
 DN 117:232345
 TI Electron impact and fast atom bombardment mass spectrometric analysis of the food-borne carcinogens 2-amino-3-methylimidazo [4,5-f] quinoline, 2-amino-3,8-dimethylimidazo [4,5-f] quinoxaline and their metabolites

AU Fay, Laurent B.; Turesky, Robert J.
 CS Nestle Res. Cent., Nestec Ltd., Lausanne, 1000, Switz.
 SO Biological Mass Spectrometry (1992), 21(9), 463-9
 CODEN: BIMSEH; ISSN: 1052-9306
 DT Journal
 LA English
 AB Electron impact (EI) and fast atom bombardment (FAB) mass spectrometry were used to characterize the heterocyclic arom. amines, 2-amino-3methylimidazo[4,5-f]quinoline and 2-amino-3,8-dimethylimidazo[4,5-f]quinoxaline and their metabolites. The carcinogenic N2-hydroxy metabolites and several non-conjugated detoxification products were analyzed directly by EI mass spectrometry, while several polar sulfate and .beta.-glucuronic acid conjugates were analyzed by FAB mass spectrometry. Anal. of .beta.-glucuronic acid conjugates was also achieved by EI mass spectrometry following silylation.

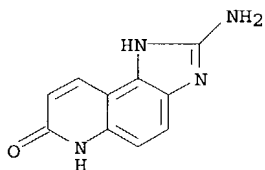
IT 108043-88-5 144240-96-0
 RL: ANT (Analyte); ANST (Analytical study)

(detn. of, in urine by mass spectrometry)

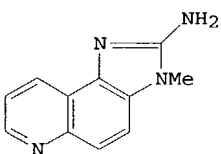
RN 108043-88-5 CAPLUS
CN 7H-Imidazo[4,5-f]quinolin-7-one, 2-amino-3,6-dihydro-3-methyl- (9CI) (CA INDEX NAME)



RN 144240-96-0 CAPLUS
CN 7H-Imidazo[4,5-f]quinolin-7-one, 2-amino-1,6-dihydro- (9CI) (CA INDEX NAME)



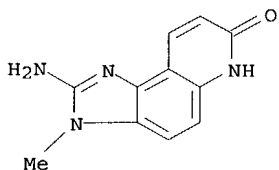
L4 ANSWER 15 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1992:628171 CAPLUS
DN 117:228171
TI Metabolism of the food mutagen 2-amino-3-methylimidazo[4,5-f]quinoline in nonhuman primates undergoing carcinogen bioassay
AU Snyderwine, Elizabeth G.; Welts, Dieter H.; Fay, Laurent B.; Wuerzner, Hans Peter; Turesky, Robert J.
CS Div. Cancer Etiol., Natl. Cancer Inst., Bethesda, MD, 20892, USA
SO Chemical Research in Toxicology (1992), 5(6), 843-51
CODEN: CRTOEC; ISSN: 0893-228X
DT Journal
LA English
GI



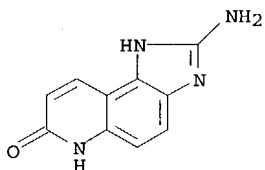
I

AB The metab. and disposition of the procarcinogen IQ (I) were investigated in monkeys undergoing carcinogen bioassay and in monkeys given an acute dose of IQ. Anal. of urine, feces, and bile revealed that IQ was extensively metabolized. Metabolites resulted from cytochrome P 450-mediated ring oxidn. at the C-5 position or N-demethylation. These metabolites could be further transformed by conjugation to sulfate or .beta.-glucuronic acid. Glucuronidation and sulfamate formation at the exocyclic amine group were other major routes of metab. Enteric bacteria also contributed to IQ biotransformation by forming the 7-oxo deriv. of IQ and N-demethyl-IQ. The metastable N2-glucuronide conjugate of the carcinogenic metabolite, 2-(hydroxyamino)-3-methylimidazo[4,5-f]quinoline, was found in urine. Thus, metabolic activation through cytochrome P 450-mediated N-oxidn. occurs in vivo and glucuronidation is a means of transport of the carcinogenic metabolite to extrahepatic tissues.

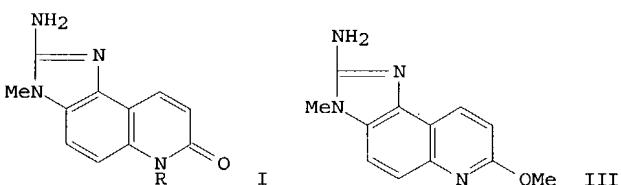
IT 108043-88-5 144240-96-0
RL: BIOL (Biological study)
(as aminomethylimidazoquinoline metabolite, in monkey)
RN 108043-88-5 CAPLUS
CN 7H-Imidazo[4,5-f]quinolin-7-one, 2-amino-3,6-dihydro-3-methyl- (9CI) (CA INDEX NAME)



RN 144240-96-0 CAPLUS
 CN 7H-Imidazo[4,5-f]quinolin-7-one, 2-amino-1,6-dihydro- (9CI) (CA INDEX NAME)



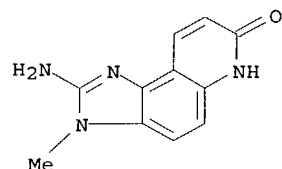
L4 ANSWER 16 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1990:440556 CAPLUS
 DN 113:40556
 TI Synthesis and biological evaluation of methylated derivatives of the cooked food mutagen metabolite 2-amino-3,6-dihydro-3-methyl-7H-imidazo[4,5-f]quinolin-7-one (7-OH-IQ)
 AU Bashir, Mohammad; Kingston, David G. I.; Van Tassell, Roger L.; Wilkins, Tracy D.
 CS Dep. Chem., Virginia Polytech. Inst. and State Univ., Blacksburg, VA, 24061-0212, USA
 SO Heterocycles (1989), 29(10), 1915-22
 CODEN: HTCYAM; ISSN: 0385-5414
 DT Journal
 LA English
 OS CASREACT 113:40556
 GI



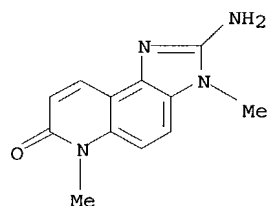
AB The major anaerobic metabolite of the potent cooked food mutagenic carcinogen IQ is the oxidized product I (R = H) (II), which is itself a powerful direct-acting mutagen. The O-Me and N-Me derivs. III and I (R = Me) of II have been prepd. to det. whether the tautomeric form of II plays any role in its bioactivity. Both I (R = Me) and III show comparable mutagenicity when tested directly against the T98 strain of Salmonella typhimurium, indicating that the quinoline structure does not play a major role in the mutagenicity of II. Neither II nor the methylated derivs. cleaved DNA in the presence of metal cations.

IT 108043-88-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (metabolites of, prepn. and mutagenicity of)

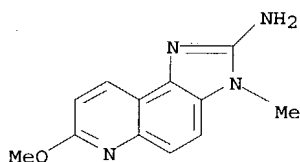
RN 108043-88-5 CAPLUS
 CN 7H-Imidazo[4,5-f]quinolin-7-one, 2-amino-3,6-dihydro-3-methyl- (9CI) (CA INDEX NAME)



IT 128006-28-0P 128006-29-1P
 RL: ADV (Adverse effect, including toxicity); SPN (Synthetic preparation);
 BIOL (Biological study); PREP (Preparation)
 (prepn. and mutagenicity of)
 RN 128006-28-0 CAPLUS
 CN 7H-Imidazo[4,5-f]quinolin-7-one, 2-amino-3,6-dihydro-3,6-dimethyl- (9CI)
 (CA INDEX NAME)



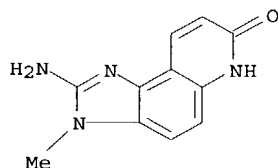
RN 128006-29-1 CAPLUS
 CN 3H-Imidazo[4,5-f]quinolin-2-amine, 7-methoxy-3-methyl- (9CI) (CA INDEX NAME)



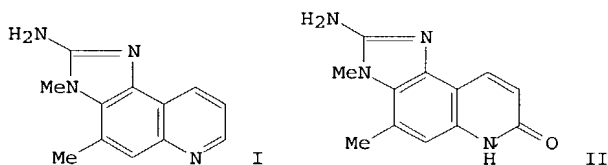
L4 ANSWER 17 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1989:626991 CAPLUS
 DN 111:226991
 TI Metabolism of 2-amino-3-methylimidazo[4,5-f]quinoline in the male rat
 AU Inamasu, T.; Luks, H.; Vavrek, M. T.; Weisburger, J. H.
 CS American Health Found., Valhalla, NY, 10595, USA
 SO Food and Chemical Toxicology (1989), 27(6), 369-76
 CODEN: FCTOD7; ISSN: 0278-6915
 DT Journal
 LA English
 AB Adult male rats were administered [2-14C]IQ or [5-3H]IQ by oral gavage at dose levels of 20 or 40 mg/kg. Rats were also given [2-14C]IQ in the diet at a dose level of 300 ppm for 2 days and after administration of unlabeled IQ (300 ppm) in the diet for approx. 6.5 wk for an addnl. 2 days. In the initial 48 h following oral administration of 20 or 40 mg [2-14C]IQ/kg, 40-50% radioactivity was recovered in the urine, and 30-38% radioactivity was recovered in the feces. In the initial 72 h following consumption of [2-14C]IQ (300 ppm) in the diet about 26% radioactivity was recovered in the urine and about 61% radioactivity was recovered in the feces. Following cannulation of the bile ducts, rats administered a single dose of [2-14C]IQ (40 mg/kg) by oral gavage excreted about 15% of the administered dose in the bile over a period of 2 days. Urine from rats given [2-14C]IQ contained three main polar metabolites that included a glucuronide, a sulfate ester and IQ sulfamate, and a no. of less polar metabolites that included IQ, 2-acetylamino-3-methylimidazo[4,5-f]quinoline, 2-aminoimidazo[4,5-f]quinoline, and 2-amino-3,6-dihydro-3-methyl-7H-imidazo[4,5-f]quinoline-7-one (7-OH-IQ). Administration of [2-14C]IQ by oral gavage or in the diet gave the same metabolites, but in different amts. In the feces of rats given [2-14C] by oral gavage, IQ sulfamate was the major metabolite in the polar fraction. Nonpolar metabolites similar to those found in the urine were also present, but in different amts. A major, nonpolar fecal metabolite, 7-OH-IQ was probably formed as a result of the activity of the intestinal bacterial flora. In rats given a single gavage dose of [2-14C]IQ, excretion of metabolites was higher in the urine and lower in the feces compared with that in animals

fed [2-14C]IQ in the diet. One polar metabolite present in the urine, IQ-sulfamate (39%), was found at considerably higher levels in rats dosed orally with IQ compared with those fed IQ (less than 6%). Thus, IQ is extensively metabolized to give a no. of polar and nonpolar metabolites, the amts. of which depend, in part, on the mode of dosing.

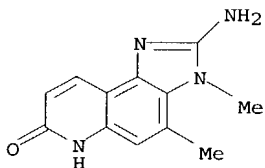
IT 108043-88-5
 RL: BIOL (Biological study)
 (as IQ metabolite, after exposure)
 RN 108043-88-5 CAPLUS
 CN 7H-Imidazo[4,5-f]quinolin-7-one, 2-amino-3,6-dihydro-3-methyl- (9CI) (CA INDEX NAME)



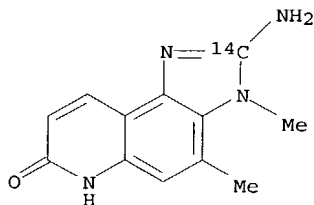
L4 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1989:550316 CAPLUS
 DN 111:150316
 TI Isolation, structure elucidation, and synthesis of the major anaerobic bacterial metabolite of the dietary carcinogen 2-amino-3,4-dimethyl-3H-imidazo[4,5-f]quinoline (MeIQ)
 AU Bashir, Mohammad; Kingston, David G. I.; Carman, Robert J.; Van Tassell, Roger L.; Wilkins, Tracy D.
 CS Dep. Chem., Virginia Polytech. Inst. and State Univ., Blacksburg, VA, 24061-0212, USA
 SO Heterocycles (1989), 29(6), 1127-35
 CODEN: HTCYAM; ISSN: 0385-5414
 DT Journal
 LA English
 GI



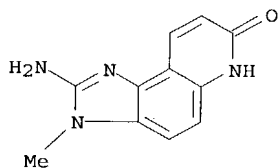
AB Incubation of the heterocyclic cooked food mutagen MeIQ (I) with mixed human fecal microflora under anaerobic conditions yielded II as the major detectable metabolite. II was synthesized in 6 steps from 6-bromo-7-methylquinoline.
 IT 122759-88-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and formation as food mutagen metabolite in anaerobic bacteria of)
 RN 122759-88-0 CAPLUS
 CN 7H-Imidazo[4,5-f]quinolin-7-one, 2-amino-3,6-dihydro-3,4-dimethyl- (9CI) (CA INDEX NAME)



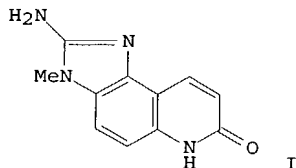
IT 122759-99-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 122759-99-3 CAPLUS
 CN 7H-Imidazo[4,5-f]quinolin-7-one-2-14C, 2-amino-3,6-dihydro-3,4-dimethyl- (9CI) (CA INDEX NAME)

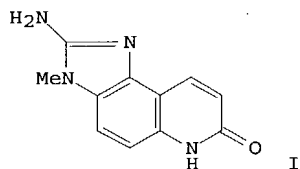


L4 ANSWER 19 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1989:90347 CAPLUS
 DN 110:90347
 TI Conversion of IQ, a dietary pyrolysis carcinogen to a direct-acting mutagen by normal intestinal bacteria of humans
 AU Carman, R. J.; Van Tassell, R. L.; Kingston, D. G. I.
 CS Dep. Anaerobic Microbiol., Virginia Polytech. Inst. and State Univ., Blacksburg, VA, 24061, USA
 SO Mutation Research (1988), 206(3), 335-42
 CODEN: MUREAV; ISSN: 0027-5107
 DT Journal
 LA English
 AB Mixed and pure cultures of human intestinal anaerobes, notably Eubacterium species, metabolized IQ to 2-amino-3,6-dihydro-3-methyl-7H-imidazo[4,5-f]quinoline-7-one (HOIQ). Unlike IQ, both the synthetic and bacterially produced HOIQ were direct-acting mutagens, i.e. active without microsomal activation. This new direct-acting mutagen, from the bacterial metab. of a dietary pyrolysis carcinogen, raises new concerns about the possible role of this class of genotoxins in the etiol. of human cancer.
 IT 108043-88-5
 RL: BIOL (Biological study)
 (IQ metab. to, by fecal bacteria and intestinal bacteria of humans, mutagenicity in relation to)
 RN 108043-88-5 CAPLUS
 CN 7H-Imidazo[4,5-f]quinolin-7-one, 2-amino-3,6-dihydro-3-methyl- (9CI) (CA INDEX NAME)



L4 ANSWER 20 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1988:422737 CAPLUS
 DN 109:22737
 TI Biological formation and chemical synthesis of 2-amino-3,6-dihydro-3-methyl-7H-imidazolo[4,5-f]quinolin-7-one, the major metabolite of the dietary carcinogen 2-amino-3-methyl-3H-imidazolo[4,5-f]quinoline (IQ) by normal intestinal bacteria
 AU Bashir, Mohammad; Kingston, David G. I.; Carman, Robert J.; Van Tassell, Roger L.; Wilkins, Tracy D.
 CS Dep. Chem., Virginia Polytech. Inst. and State Univ., Blacksburg, VA, 24061, USA
 SO Heterocycles (1987), 26(11), 2877-86
 CODEN: HTCYAM; ISSN: 0385-5414
 DT Journal
 LA English
 OS CASREACT 109:22737
 GI



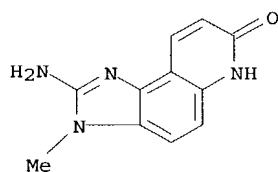


AB 2-Amino-3,6-dihydro-3-methyl-7H-imidazo[4,5-f]quinolin-7-one (I) has been synthesized from 6-bromo-5-nitroquinoline in 7 steps. Biol. formation of I from IQ involves the addn. of H₂O from the medium, followed by oxidn.

IT 108043-88-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(microbial formation from IQ and prepn. of)

RN 108043-88-5 CAPLUS

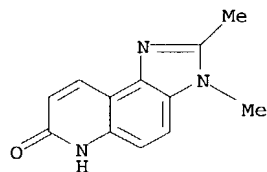
CN 7H-Imidazo[4,5-f]quinolin-7-one, 2-amino-3,6-dihydro-3-methyl- (9CI) (CA INDEX NAME)



IT 115071-63-1P 115091-26-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

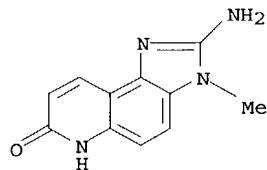
RN 115071-63-1 CAPLUS

CN 7H-Imidazo[4,5-f]quinolin-7-one, 3,6-dihydro-2,3-dimethyl- (9CI) (CA INDEX NAME)



RN 115091-26-4 CAPLUS

CN 7H-Imidazo[4,5-f]quinolin-7-one, 2-amino-3,6-dihydro-3-methyl-, monohydrobromide (9CI) (CA INDEX NAME)



● HBr

L4 ANSWER 21 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1987:190840 CAPLUS

DN 106:190840

TI Anaerobic metabolism of 2-amino-3-methyl-3H-imidazo[4,5-f]quinoline (IQ) by human fecal flora

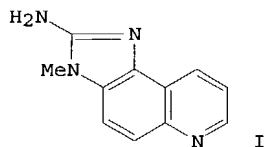
AU Bashir, M.; Kingston, D. G. I.; Carman, R. J.; Van Tassell, R. L.; Wilkins, T. D.

CS Virginia Polytech. Inst. and State Univ., Blacksburg, VA, 24061, USA

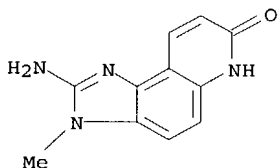
SO Mutation Research (1987), 190(3), 187-90

CODEN: MUREAV; ISSN: 0027-5107

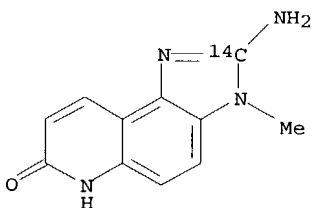
DT Journal
LA English
GI



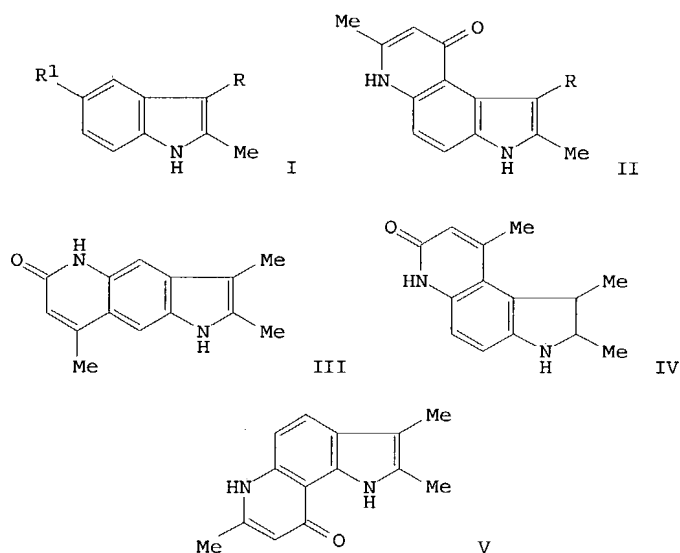
AB Incubation of the heterocyclic cooked food mutagen IQ (I) [76180-96-6] with mixed human fecal microflora under anaerobic conditions yielded 2-amino-3,6-dihydro-3-methyl-7H-imidazo[4,5-f]quinolin-7-one (II) [108043-88-5] as the major detectable metabolite.
IT 108043-88-5
RL: BIOL (Biological study)
(as IQ metabolite, after anaerobic metab. by human fecal flora)
RN 108043-88-5 CAPLUS
CN 7H-Imidazo[4,5-f]quinolin-7-one, 2-amino-3,6-dihydro-3-methyl- (9CI) (CA INDEX NAME)



IT 108026-25-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 108026-25-1 CAPLUS
CN 7H-Imidazo[4,5-f]quinolin-7-one-2-14C, 2-amino-3,6-dihydro-3-methyl- (9CI) (CA INDEX NAME)



L4 ANSWER 22 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:438395 CAPLUS
DN 99:38395
TI Synthesis of pyrroloquinolones
AU Yamashkin, S. A.; Yudin, L. G.; Kost, A. N.
CS Mosk. Gos. Univ., Moscow, USSR
SO Khimiya Geterotsiklicheskikh Soedinenii (1983), (4), 493-7
CODEN: KGSSAQ; ISSN: 0453-8234
DT Journal
LA Russian
OS CASREACT 99:38395
GI

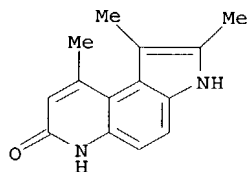


AB Intramol. cyclocondensation of I (R = Me, H; R1 = EtO2CCH:CMenH) by refluxing in biphenyl gave 89 and 95% pyrroloquinolines II. Similarly, refluxing I (R = Me, R1 = MeCOCH2CONH) in F3CCO2H gave a mixt. contg. III and IV. Refluxing I (R = Me, R1 = EtO2CCH:CMenH in the 6 position) with biphenyl gave 90% V.

IT 86269-88-7P 86269-91-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

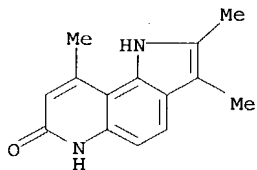
RN 86269-88-7 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2,9-trimethyl- (9CI) (CA INDEX NAME)



RN 86269-91-2 CAPLUS

CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 1,6-dihydro-2,3,9-trimethyl- (9CI) (CA INDEX NAME)



L4 ANSWER 23 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1982:6616 CAPLUS

DN 96:6616

TI Chichibabin reaction in a series of angular pyrroloquinolines

AU Akhvlediani, R. N.; Shabunova, V. P.; Morozova, I. A.; Volodina, T. A.; Suvorov, N. N.

CS Khim.-Tekhnol. Inst., Moscow, USSR

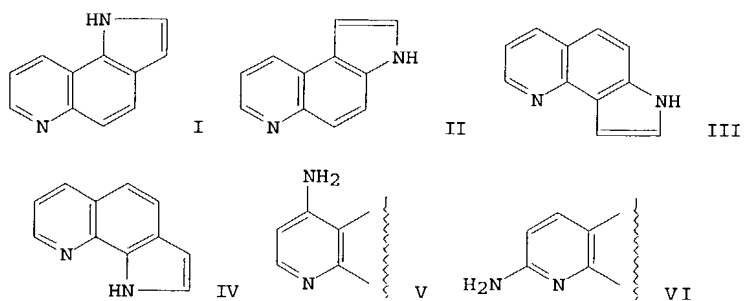
SO Zhurnal Organicheskoi Khimii (1981), 17(7), 1542-6
 CODEN: ZORKAE; ISSN: 0514-7492

DT Journal

LA Russian

OS CASREACT 96:6616

GI



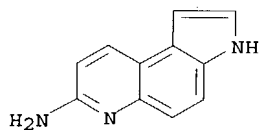
AB The angular pyrroloquinolines I, II, III and IV, underwent amination with NaNH_2 in xylene at the .alpha. and .gamma. positions to give mixts. of amino derivs. V and VI.

IT 80077-05-0P 80104-38-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 80077-05-0 CAPLUS

CN 3H-Pyrrolo[3,2-f]quinolin-7-amine (9CI) (CA INDEX NAME)



RN 80104-38-7 CAPLUS

CN 1H-Pyrrolo[2,3-f]quinolin-7-amine (9CI) (CA INDEX NAME)

